Inelastic Confinement-Induced Resonances in Low-Dimensional Quantum Systems

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A theoretical model is presented describing the confinement-induced resonances observed in the recent loss experiment of Haller et al. [Phys. Rev. Lett. 104, 153203 (2010)]. These resonances originate from possible molecule formation due to the coupling of center-of-mass and relative motion. A corresponding model is verified by ab initio calculations and predicts the resonance positions in 1D as well as in 2D confinement in agreement with the experiment. This resolves the contradiction of the experimental observations to previous theoretical predictions.

Low-dimensional quantum systems show intriguing phenomena. For example, a 2D confinement allows for the existence of particles with fractional statistics known as anyons [1]. In 1D a gas of impenetrable Bosons, the Tonks-Girardeau gas, acquires Fermionic properties [2, 3]. Nowadays, one and two-dimensional systems can be experimentally realized in trapped ultracold gases offering a high degree of control [2, 4, 5]. In low-dimensional systems confinement-induced resonances (CIRs) have attracted great interest. They are universal, since they depend solely on the geometry of the trap. In 1998, Olshanii developed a mapping of the relative-motion Hamiltonian of a system of two atoms confined in a harmonic trap at large anisotropies onto the corresponding purely one-dimensional one [6]. The resulting 1D effective interaction strength g_{1D} shows a divergent behavior at a specific scattering length which leads to the formation of a Tonks-Girardeau gas [7, 8]. An analogous derivation of the effective 2D interaction strength g_{2D} reveals a similar divergent behavior [9]. The divergences in these models, which are based on the relative-motion Hamiltonian in harmonic approximation (RMH models), were confirmed in 1D by ab initio calculations of g_{1D} [10] and very recently in 2D adopting radio-frequency spectroscopy to measure g_{2D} [11]. An experimental search for the predicted CIRs in terms of particle losses and heating was performed by Haller *et al.* [5]. In 1D, a resonance close to the position predicted by the RMH model was found for isotropic transversal confinement. However, the experiment considered also an anisotropic transversal confinement and found an unexpected splitting of the resonance. Furthermore, in 2D confinement a resonance was observed at positive values of the scattering length. A detailed analysis [12] proved formally that these two observations contradict the RMH models that predict a *single* resonance in 1D and a resonance at *negative* scattering lengths in 2D confinement. The immediate question arises what kind of resonances were observed in [5]. Are the RMH resonances modified due to the experimental setup, or are the losses in [5] of completely different origin? If so, why are RMH resonances not seen in terms of losses?

In this Letter it will be demonstrated that the resonances observed in [5] are caused by a coupling of the center-of-mass (COM) and relative (REL) motion which originates from the anharmonic terms of the trapping optical lattice. The COM-REL coupling (CRC) and strong 1D or 2D confinement leads to Feshbach resonances induced by (avoided) crossings of bound states with COM excitation and a state of an unbound atom pair without COM excitation. Hence, at the avoided crossing a molecular bound state can be occupied, since the excess binding energy can be transferred to COM excitation energy. In view of this energy transfer we refer to the COM-REL resonance as an *inelastic* CIR. The formation of molecules is a basic loss mechanism and should thus be observable in loss experiments like [5]. On the contrary, in the spectra of the RMH Hamiltonians [13] no curve crossings appear that could lead to a significant occupation of an excited bound state and corresponding molecule formation [14]. Because of the absence of an energy transfer the CIRs of the RMH models are denoted as *elastic* CIRs in the following.

The CRC model is introduced, first for 1D and later for 2D confinement, for two identical particles in agreement with the experiment. The external potential is assumed to be expandable in a power series around the origin and separable in the three spatial directions. In COM and REL coordinates, $\mathbf{r} = \mathbf{r_1} - \mathbf{r_2}$ and $\mathbf{R} = \frac{1}{2}(\mathbf{r_1} + \mathbf{r_2})$, the Hamiltonian is given as

$$H(\mathbf{r},\mathbf{R}) = T_{\mathrm{REL}}(\mathbf{r}) + T_{\mathrm{COM}}(\mathbf{R}) + V_{\mathrm{REL}}(\mathbf{r}) + V_{\mathrm{COM}}(\mathbf{R}) + U_{\mathrm{int}}(r) + W(\mathbf{r},\mathbf{R}) \quad (1)$$

where T_{REL} and T_{COM} are the kinetic-energy operators of the REL and COM motion, respectively. V_{REL} and V_{COM} are the separable parts of the potential energy. Thus, W contains only the non-separable terms that are of the form $r_i^n R_i^m$ with $i \in \{x, y, z\}$ and $n, m \in \mathbb{N}\backslash\{0\}$. $U_{\mathrm{int}}(r)$ is the inter-particle interaction which in the CRC model is described by the pseudo potential $U_{\mathrm{int}}(r) = \frac{4\pi\hbar^2 a}{m}\delta(\mathbf{r})\frac{\partial}{\partial r}r$ where a is the 3D s-wave scattering length and m the atom mass. In the case of an optical lattice in three spatial directions the external potential terms read

$$V_{\mathrm{REL}}(\mathbf{r}) = 2\sum_{j=x,y,z} V_j \sin^2(\frac{1}{2}kr_j) \quad (2)$$

$$V_{\rm COM}(\mathbf{R}) = 2\sum_{j=x,y,z} V_j \sin^2(kR_j) \tag{3}$$

$$W(\mathbf{r},\mathbf{R}) = -4\sum_{j=x,y,z} V_j \sin^2(\frac{1}{2}kr_j)\sin^2(kR_j) \tag{4}$$

with $k=\frac{2\pi}{\lambda}$ and λ the laser wavelength. V_j is the lattice depth in direction $j\in\{x,y,z\}$. In an optical lattice 1D geometry can be achieved by forming decoupled quasi 1D tubes which requires a sufficient lattice depth in two transversal directions, e.g., x and y. Consequently, it suffices to consider the physics of a single tube.

To estimate the energy spectrum the harmonic approximation of a single tube with trap frequencies ω_j and trap lengths $d_j=\sqrt{2\hbar/(m\omega_j)}$ is considered. The confinement is characterized by the anisotropies $\eta_x=\omega_x/\omega_z$ and $\eta_y=\omega_y/\omega_z$, which should be sufficiently large. Within the harmonic approximation the coupling between COM and REL motion vanishes. The wavefunctions are thus represented by products of COM and REL eigenstates. The harmonic relative motion Hamiltonian possesses a single bound state $\psi^{(b)}(\mathbf{r})$ [15]. The influence of the weak longitudinal confinement on the bound state energy $E_b^{\rm REL}(a)$ can be neglected [13]. In this case $E_b^{\rm REL}$ and a satisfy the relation [12]

$$\frac{\sqrt{\pi}d_y}{a} = -\int_0^\infty \left(\frac{\sqrt{\beta}\,\mathrm{e}^{\frac{t\epsilon}{2}}}{\sqrt{t\,(1-\mathrm{e}^{-\beta\,t})\,(1-\mathrm{e}^{-t})}} - t^{-\frac{3}{2}}\right)dt \tag{5}$$

where $\epsilon=(E_b^{\rm REL}-E_0)/(\hbar\omega_y)$, $E_0=\frac{\hbar}{2}(\omega_x+\omega_y)$, and $\beta=\omega_x/\omega_y$. A general expression for the eigenenergies above the REL motion threshold $E_{\rm th}=\frac{\hbar}{2}(\omega_x+\omega_y+\omega_z)$ is not known. The states above $E_{\rm th}$ are denoted as trap states in the following. The eigenenergy $E_1^{\rm REL}$ of the first trap state $|\psi_1\rangle$ lies in the interval $[E_{\rm th},E_{\rm th}+2\hbar\omega_z)$ such that for the model $E_1^{\rm REL}$ is approximated by $E_{\rm th}+\hbar\omega_z$ [16]. In the limit as the temperature $T\to 0$, the higher excitations are frozen out. The eigenstates of the COM Hamiltonian factorize as $\Phi_{\mathbf{n}}(\mathbf{R})=\phi_{n_x}(X)\,\phi_{n_y}(Y)\,\phi_{n_z}(Z)$ with $\mathbf{n}=(n_x,n_y,n_z)$ and eigenenergies $E_{\mathbf{n}}^{\rm COM}=\sum_{j=x,y,z}\hbar\omega_j(n_j+\frac{1}{2})$. When combining REL and COM motion the energies of the bound states become $E_b^{\rm REL}(a)+E_{\mathbf{n}}^{\rm COM}$ while the energy of the lowest trap state is given by $E_1^{\rm REL}+E_{(0,0,0)}^{\rm COM}$. For $n\neq(0,0,0)$ *crossings* between the excited bound state and the lowest trap state occur for

$$E_b^{\rm REL} = E_1^{\rm REL} - \Delta_{\mathbf{n}} \tag{6}$$

where $\Delta_{\mathbf{n}}=E_{\mathbf{n}}^{\rm COM}-E_{(0,0,0)}^{\rm COM}$ is the COM excitation. The corresponding scattering length at the crossing is obtained from Eq. (5).

In the following, the influence of the anharmonicity of the confining potentials of Eqs. (2), (3), and (4) is considered. First of all, the non-vanishing term $W(\mathbf{r},\mathbf{R})\neq 0$ leads to the coupling between REL and COM states of equal symmetry. Resonances are only observable if the coupling between the crossing states is sufficiently strong. Within the CRC model, the matrix elements defining the coupling strength between a bound state $|\Phi_{\mathbf{n}}\,\psi^{(b)}\rangle$ with COM excitation $\Delta_{\mathbf{n}}$ and the lowest trap state $|\Phi_{(0,0,0)}\,\psi_1\rangle$ are $W_{\mathbf{n}}=\langle\Phi_{\mathbf{n}}\,\psi^{(b)}|W|\psi_1\,\Phi_{(0,0,0)}\rangle$. Since $W(\mathbf{r},\mathbf{R})=\sum_{j=x,y,z}W_j(r_j,R_j)$ separates in the spatial directions the matrix elements become

$$W_{\mathbf{n}} = \sum_{j=x,y,z}\langle\Phi_{\mathbf{n}}\,\psi^{(b)}|W_j|\Phi_{(0,0,0)}\,\psi_1\rangle. \tag{7}$$

The coupling to a bound state along the weakly confined z direction can be neglected, because the bound state has an extension $d_b\ll d_z$. Hence, $W(z,Z)\approx W(0,Z)$ holds within the extension of the bound state $|z|\leq d_b$ and due to the orthogonality of the REL eigenstates the longitudinal matrix element vanishes, $\langle\Phi_{\mathbf{n}}\psi^{(b)}|W_z|\psi_1\Phi_{(0,0,0)}\rangle\approx\langle\Phi_{\mathbf{n}}|W_z(z=0,Z)|\Phi_{(0,0,0)}\rangle\langle\psi^{(b)}|\psi_1\rangle=0$. With this approximation the coupling matrix element (7) becomes

$$W_{\mathbf{n}} \approx \delta_{n_z,0}\times\Big[\delta_{n_y,0}\langle\phi_{n_x}\psi^{(b)}|W_x|\psi_1\phi_0\rangle + \delta_{n_x,0}\langle\phi_{n_y}\psi^{(b)}|W_y|\psi_1\phi_0\rangle\Big]. \tag{8}$$

As implied by Eq. (6), the excitation of the bound state $\Delta_{\mathbf{n}}$ must be nonzero for crossings to exist. It follows directly from Eq. (8) that resonances can only occur for excitations of the bound state in a *single transversal* direction. For symmetry reasons the excitations must be even. The couplings connected to the lowest transversal excitations are dominant, because for higher excitations the increasing oscillatory behavior of the wavefunctions reduces the values of the integrals in Eq. (8). Hence, the inelastic CIRs for the quasi 1D confinement arise dominantly from the coupling matrix elements with quantum numbers $n=(2,0,0)$ and $n=(0,2,0)$.

Based on these selection rules the positions of the inelastic CIR can be predicted. So far, the harmonic approximation is used to determine the energy crossings. For the excitations of the bound state higher COM states are involved so that the influence of the anharmonicity on the COM energy cannot be neglected. Therefore, $\Delta_{\mathbf{n}}$ in Eq. (6) is corrected within first-order perturbation theory treating the leading anharmonic (quartic) term of the COM optical lattice, $-\frac{1}{24}\sum_{j=x,y,z}\frac{\hbar\omega_j}{V_j}R_j^4$, as a perturbation. The resulting energy offset $\Delta_{\mathbf{n}}$ becomes

$$\Delta_{(n_x,n_y,n_z)} = \sum_{j=x,y,z}\hbar\omega_j n_j\left(1-\frac{\hbar\omega_j}{16V_j}\left[n_j+1\right]\right). \tag{9}$$

The CIR positions can now be easily determined using Eqs. (6) and (9) with $n=(2,0,0)$ and $n=(0,2,0)$. Figure 1 shows that the predicted resonance positions agree perfectly to the experimental positions of maximal

atom loss. Note, while in [5] the "edges", i.e. the scattering length for which the atom loss starts to rise significantly, were chosen as resonances positions, in the CRC model the conventional positions of maximal particle loss are considered [17]. The CRC model explains accurately the observed splitting of the resonance for anisotropic transversal confinement.

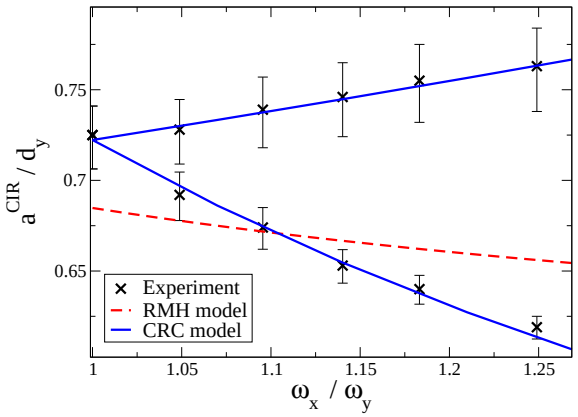

Figure 1. (color online) Positions of CIRs in terms of the scattering length for different values of transversal anisotropy in quasi 1D. The experimental positions of maximal particle loss are compared to the predicted CIR positions of the RMH model and the CRC model using the experimental parameters (Cs atoms confined in a trap with $\eta_y = 825$, $V_y = 24.8E_r$ and $\lambda = 1064.49$ nm where $E_r = \hbar^2k^2/2m$ is the photon recoil energy.

In the following full *ab initio* calculations of the spectrum of the general Hamiltonian (1) are presented to validate the CRC model. The calculations are performed by a full six-dimensional exact-diagonalization approach which uses a basis of B splines and spherical harmonics [18]. To incorporate coupling, sextic potentials are used which are an accurate representation of a single site of an optical lattice [18]. The interaction is described by a Born-Oppenheimer potential which can be varied to tune the scattering length a to arbitrary values [18]. While in the experiment a quasi 1D trap of large anisotropy with $\eta_x \approx \eta_y \approx 900$ is used, the calculations are performed with $\eta_x \approx \eta_y = 10$ which is however already well in the quasi 1D regime [13]. Larger anisotropies would lead to a prohibitive computational effort. A fully coupled spectrum for transversal isotropy ($\eta_x = \eta_y$) is shown in Fig. 2. The complex structure of the energy spectrum is highlighting the importance of the derived selection rules that specify which of the crossing states couple significantly. The coupling strength is proportional to the width of the avoided crossings that can be observed in Fig. 3 and the lower graph of Fig. 2. The selection rules are clearly verified: significant avoided crossings appear only for transversally excited bound states whereas a longitudinal excitation leads to negligible coupling.

While in the case of isotropic confinement, $\eta_x = \eta_y$,

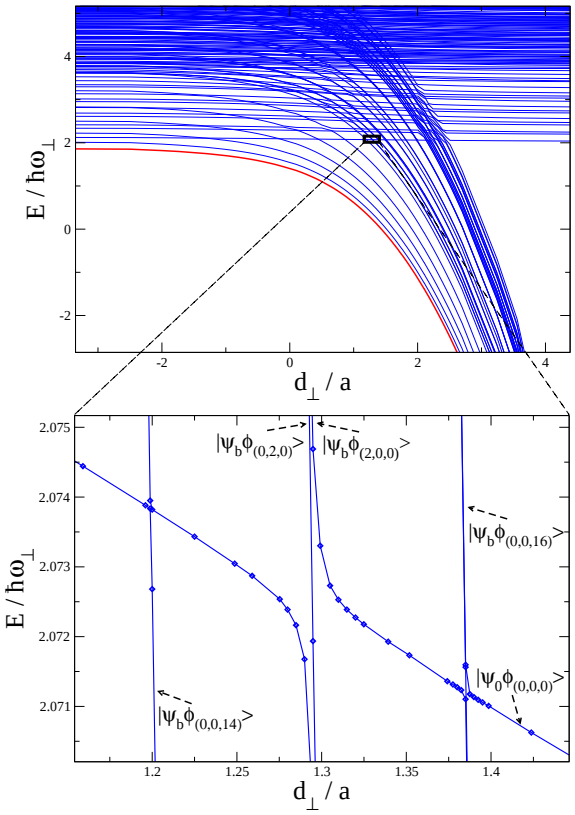

Figure 2. (color online) Spectrum of the full coupled Hamiltonian (1) for ^{7}Li atoms confined in a sextic trapping potential with $V_x = V_y = 35.9E_r$, $\eta_x = \eta_y = 10$ and $\lambda = 1000$ nm. In the upper part all states bending down to $-\infty$ are molecular states originating from the REL bound state $\psi^{(b)}$ with different COM excitations. The one in the COM ground state is marked red. The magnified part shows the avoided crossing responsible for the inelastic CIR which arises from the crossings of the transversally excited bound states with the ground trap state. The kets indicate the dominant contribution to the states. Only transversally excited states couple strongly while for longitudinal excitation the coupling is very small resulting in almost non-avoided crossings. For isotropic transversal confinement only one CIR occurs due to the degeneracy of the transversal excitation.

the transversally excited states are degenerate and only a single resonance is visible, for anisotropic confinement, $\eta_x \neq \eta_y$, this degeneracy is lifted. In accordance with the CRC model a splitting of the CIR positions appears in Fig. 3. In Fig. 4 the CIR positions of the *ab initio* calculations and the CRC model are shown. The stronger longitudinal confinement results in a systematic shift of the resonances towards larger values of the scattering length. This is mainly caused by the behavior of the energy of the first trap state. Although this energy could only be estimated within the CRC model the deviations to the *ab initio* results are less than 1%. In contrast, the resonance position of the elastic CIR predicted by the RMH model is independent of the longitudinal confinement.

Next, the CRC model is extended to 2D confinement

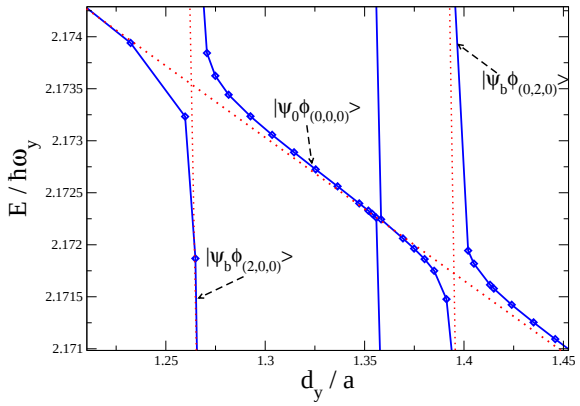

Figure 3. (color online) Spectrum of the full coupled Hamiltonian (1) for ^{7}Li atoms confined in a sextic trapping potential with $V_y = 35.9E_r$, $\eta_x = 11$, $\eta_y = 10$ and $\lambda = 1000$ nm. The kets indicate the dominant contribution to the states. Only transversally excited bound states couple strongly to the ground trap state as displayed by the size of the avoided crossing. The two CIRs correspond to COM excitations in either of the transversal directions.

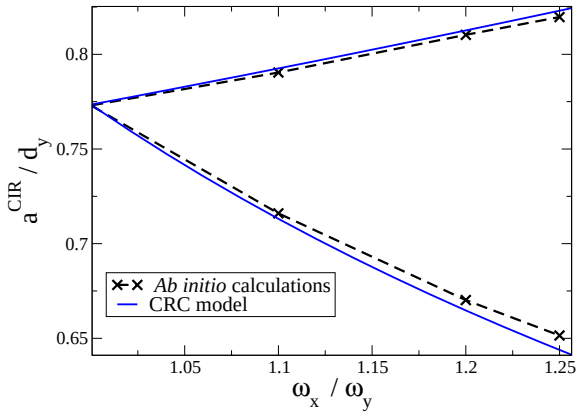

Figure 4. (color online) Positions of inelastic CIRs for different values of the transversal anisotropy in quasi 1D. The results of the *ab initio* calculations are compared to the prediction of the CRC model using the same parameters (^{7}Li atoms confined in a sextic trapping potential with $V_y = 35.9E_r$, $\eta_y = 10$ and $\lambda = 1000$ nm) that, however, differ from the ones in Fig. 1.

which is characterized by a single strong transversal confinement in, e.g., the x direction (i.e. $\omega_x \gg \omega_y, \omega_z$). While Eq. (5) and Eq. (6) stay valid, the contributions of the weakly confined directions to the matrix element in Eq. (7) can be neglected. Hence, the coupling matrix element between an excited bound state and the lowest trap state becomes

$$W_{\mathbf{n}} \approx \delta_{n_y,0}\delta_{n_z,0}\langle\phi_{n_x}\psi^{(b)}|W_x|\psi_1\phi_0\rangle. \qquad (10)$$

Only a transversally excited bound state with $n_x = 2, 4, \ldots$; $n_y = n_z = 0$ can lead to coupling. Again, only the first excitation $\mathbf{n} = (2, 0, 0)$ is dominant, i.e. only a single resonance appears. In the experiment [5] a single resonance is observed for 2D confinement indicated by maximal particle loss at $\frac{a}{d_y} = 0.593$ [19]. For the experimental trap parameters the CRC model predicts the CIR at $\frac{a}{d_y} = 0.595$, again, in perfect agreement. This highlights the fundamental difference to the RMH model which predicts a resonance for *negative* values of the scattering length in 2D confinement.

As in the 1D case the selection rules of the CRC model are confirmed by full *ab initio* calculations. For $\eta_x = 10$ and $\eta_y = 1$ both the *ab initio* calculations and the CRC model predict the CIR position at $\frac{a}{d_y} = 0.64$ showing again that the resonance position depends also on the strength of the weak confinement.

In conclusion, a model describing inelastic CIRs is presented which explains qualitatively and quantitatively the surprising experimental results of a splitting of the resonance under transversal anisotropic 1D confinement and a resonance at positive scattering length in 2D confinement in the loss experiment [5]. These resonances are caused by the coupling to bound states with COM excitation in the tightly confined direction. At the inelastic CIR molecules are formed causing enhanced losses. The previously known CIRs are elastic and are therefore hardly visible in a loss experiment. However, they can be observed by measuring the effective interaction strength directly [11]. The model has important consequences for the experimental realization of a Tonks-Girardeau gas. As the inelastic-resonance position depends sensitively on the energy of the resonant excited bound state, it is possible to prepare a system on the broad elastic CIR where $g_{1D} \to \infty$, i.e. the Tonks-Girardeau limit is reached, while being off resonant to the excited bound state and thus avoiding atom losses [2]. In 2D the elastic and inelastic CIRs are well separated which explains the different resonance positions observed in [5] and [11]. Since the underlying mechanism of COM-REL coupling leading to an inelastic CIRs is of very general nature, we believe that they can be observable in various physical systems.

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